Abstract: Cross sections for ionization of inner-shell electrons by electron impact*

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Auger electron spectroscopy (AES) has been used extensively for qualitative surface analyses in recent years. There have, however, been relatively few attempts at quantitative surface analyses on account of lack of knowledge of key parameters (such as electron attenuation lengths, inner-shell ionization cross sections, and backscattering factors) as a function, where appropriate, of material, incident electron energy, Auger electron energy, and instrumental characteristics. A review of experimental electron attenuation length data in the energy range relevant to AES and to x-ray photoelectron spectroscopy (XPS) was given in a previous paper[1] together with a method to predict attenuation lengths in other materials. We give a summary here of an analysis[2] of available data concerning cross sections for ionization of inner-shell electrons by electron impact. Cross-section data of this type is also required in correction procedures for quantitative analysis by electron probe microanalysis.[3] Unfortunately, the data base is limited, so of necessity the analysis has been limited to K- and L-shell ionization of light atoms.

Calculated, semiempirical, and experimental cross-section data have been intercompared graphically and through fits to the linearized Bethe equation[4,5] for inner-shell ionization. The Bethe equation is

$$\sigma_{nl} = (2\pi e^4/mv^2 E_{nl}) Z_{nl}\, b_{nl} \ln(2mv^2/B_{nl}), \quad (1)$$

where $E_0 = mv^2/2$ is the energy of the incident electron beam, E_{nl} is the binding energy of electrons in the nl-shell, and Z_{nl} is the number of electrons in that shell. The parameter b_{nl} was estimated by Bethe to be between 0.2 and 0.6 and the parameter B_{nl} to be of the order of E_{nl}. In the derivation of Eq. (1) it has been assumed that $E_0 \gg E_{nl}$ and it then becomes important to ask, as a practical matter, what is the lowest value of E_0 for which Eq. (1) will be valid?

It is convenient to write Eq. (1) in the form

$$\sigma_{nl} E_{nl}^2 = 6.51\times10^{-14} Z_{nl}\, b_{nl} \ln(c_{nl} U_{nl})/U_{nl} \quad \mathrm{cm^2 eV^2}, \quad (2)$$

where $c_{nl} = 4E_{nl}/B_{nl}$ and where the energy E_{nl} has been expressed in eV. Calculated and measured cross-section data can be used to find "effective" values of the Bethe parameters b_{nl} and c_{nl} to test, first, the range of validity of Eq. (1) for a particular element and a particular inner shell and, second, the possible variation of the parameters b_{nl} and c_{nl} with Z (for a particular shell). The Bethe parameters can be obtained conveniently from a linear least-squares fit to the following equation (a Fano plot[5])

$$\frac{\sigma_{nl} E_{nl}^2 U_{nl}}{6.51\times10^{-14}\, Z_{nl}} = b_{nl} \ln U_{nl} + A_{nl}, \quad (3)$$

where

$$A_{nl} = b_{nl} \ln c_{nl}.$$

Almost all of the available data can be satisfactorily fitted over the range $4 \lesssim U_{nl} \lesssim 30$ and values obtained for the effective parameters b_{nl} and c_{nl}.[2] Values of the parameter b_{nl} have also been derived from photoabsorption data and were found to be consistent with the ionization data if account was taken of the distribution of differential oscillator strength with respect to excitation energy. Specifically, b_{nl} should properly be regarded as a function of U_{nl} for $U_{nl} \lesssim 20$ although useful empirical fits to the cross-section data can be obtained over a wide range of U_{nl}, as mentioned above, with a different (higher) effective value of b_{nl} and a lower than expected value of c_{nl}. The derived empirical Bethe parameters should therefore not be used outside the range of each fit.

Experimental values of $\sigma_K E_K^2$ appeared to lie on a common curve when plotted as function of U_K. These values agreed quite well with the theoretical results of Rudge and Schwartz[6] for $5 < U_K < 26$ and the results of McGuire.[7] It therefore appears that values of σ_K for light atoms can be obtained by appropriate scaling.

A greater spread existed in the plot of calculated and measured values of $\sigma_{L_{23}} E_{L_{23}}{}^2$ as a function of $U_{L_{23}}$ than for the case of K-shell ionization. A significant variation in the magnitude of $\sigma_{L_{23}} E_{L_{23}}^2$ as a function of Z (for a given value of $U_{L_{23}}$) is apparent in the experimental data of Vrakking and Meyer[8] and in the calculations of McGuire.[7] This variation leads to a large variation in the magnitude of the effective $b_{L_{23}}$ as a function of Z that is not substantiated by the results of many photoabsorption experiments or by the limited number of L-shell ionization cross sections derived from characterization x-ray and Auger electron yield experiments. Further experiments are required to resolve this discrepancy.

Although the data base in the range of interest here is limited, it is possible to provide "preferred values" for the empirical Bethe parameters. For the case of K-shell ionization, the values $b_K \sim 0.9$ and

$c_K \sim 0.60$–0.75 appear to be useful for light atoms in the range $4 < U_K < 25$. The situation for L_{23}-shell ionization is less certain, for the reasons just discussed, but the values $b_{L_{23}} \sim 0.5$–0.6 nd $c_{L_{23}} \sim 1$ seem reasonable choices for $U_L \gtrsim 20$, while the values $c_{L_{23}} \sim 0.6$–0.9 and $U_{L_{23}} \sim 0.6$ seem reasonable for $4 < U_L$ 23 $\lesssim 20$.

The relatively simple and widely used expressions of Gryzinski,[9] Drawin,[10] and Lotz[11] agree closely with each other (within 10%) in the case of K-shell ionization for $U_K < 30$. These results are systematically lower than the experimental measurements by roughly 10% to 15%. For the case of L_{23}-shell ionization, the Lotz expression is substantially different from the Gryzinski and Drawin results (which agree well with each other). The latter results agree closely with the cross-section measurements of Christofzik[12] for argon.

The principal conclusions of the analysis are as follows:

(a) Useful empirical fits of inner-shell ionization cross-section data can be made with Eqs. (1) to (3) over a wide range of U_{nl} (typically $4 \lesssim U_{nl} \lesssim 30$) with effective values of the Bethe parameters b_{nl} and c_{nl}. The effective value of b_{nl} is consistent with photoabsorption data taking into account the anticipated functional dependence of b_{nl} on E_0.

(b) The present data base does not indicate a significant variation of the Bethe parameters with Z.

(c) A better choice of the Bethe parameters can be made now than those recommended many years ago by Mott and Massey.[13] The recent calculations and measurements show that the inner-shell ionization cross sections are appreciably (at least 40% to 50%) higher than those calculated with the Mott and Massey parameters.

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